

October 4, 2002

Doug Anderson
Panel Manager
The American Chemistry Council
Higher Olefins Panel
1300 Wilson Boulevard
Arlington, VA 22209

Dear Mr. Anderson:

The Office of Pollution and Toxics is transmitting EPA's comments on the robust summaries and test plan for the Higher Olefins Category posted on the ChemRTK HPV Challenge Program Web site on October 22, 2001. I commend The American Chemistry Council Higher Olefins Panel for its commitment to the HPV Challenge Program.

EPA reviews test plans and robust summaries to determine whether the reported data and test plans will provide the data necessary to adequately characterize each SIDS endpoint. On its Challenge Web site, EPA has provided guidance for determining the adequacy of data and preparing test plans used to prioritize chemicals for further work.

EPA will post this letter and the enclosed Comments on the HPV Challenge Web site within the next few days. As noted in the comments, we ask that The American Chemistry Council Higher Olefins Panel advise the Agency, within 90 days of this posting on the Web site, of any modifications to its submission.

If you have any questions about this response, please contact Richard Hefter, Chief of the HPV Chemicals Branch, at 202-564-7649. Submit questions about the HPV Challenge Program through the HPV Challenge Program Web site "Submit Technical Questions" button or through the TSCA Assistance Information Service (TSCA Hotline) at (202) 554-1404. The TSCA Hotline can also be reached by e-mail at tsca-hotline@epa.gov.

I thank you for your submission and look forward to your continued participation in the HPV Challenge Program.

Sincerely,

-S-

Oscar Hernandez, Director
Risk Assessment Division

Enclosure

cc: C. Auer
A. Abramson
W. Penberthy
M. E. Weber

**EPA Comments on Chemical RTK HPV Challenge Submission:
Higher Olefins Category**

SUMMARY OF EPA COMMENTS

The sponsor, the American Chemistry Council Higher Olefins Panel, submitted a test plan and robust summaries to EPA for the Higher Olefins category dated July 2001. EPA posted the submission on the ChemRTK HPV Challenge website on October 22, 2001. The Higher Olefins category includes olefins with even and odd carbon numbers, linear and branched alkyl chains, and internal and terminal olefins covered under 30 CAS number designations.

EPA has reviewed this submission and has reached the following conclusions:

1. Category Justification. EPA generally agrees with the submitter's approach for grouping the chemicals under this category and agrees that the incremental changes in the carbon number (C₆-C₅₄) across the category are reflected in the physicochemical/environmental properties and the toxicities of the category members. The submitter needs to address several issues in order to justify the approach adequately.
2. Physicochemical Properties and Environmental Fate Data. (a) The submitter provided estimated values for water solubility and log K_{ow}, and proposes providing calculated data for the remaining physicochemical properties. The submitter needs to provide measured data for boiling point, vapor pressure and water solubility for representative chemicals within the category. (b) The submitter needs to provide biodegradation data for those alpha olefins with molecular weights ranging from C₃₀ to C₅₄. (c) EPA agrees with the submitter's plan to provide data for photodegradation, transport and distribution, and a technical discussion for stability in water.
3. Health Endpoints. With the exception of repeated-dose and reproductive/developmental toxicity, the submitted data are adequate for the purposes of the Challenge Program. The submitter proposes conducting a 28-day combined repeated-dose/reproductive/developmental toxicity screening test on a C₆ internal olefin stream to address these endpoints at the lower end of the series. In addition, for higher molecular weight materials, the submitter proposes conducting a reproductive/developmental toxicity screening test on a C₁₈, mostly linear internal olefin. EPA agrees with this approach.
4. Ecological Effects. The robust summaries were either deficient or inadequate and those based on useful studies need to be revised. EPA agrees with the submitter's plan to conduct acute invertebrate and algal toxicity testing on a C₆ internal olefin. EPA believes that a chronic daphnia reproduction test should also be done on another hydrophobic internal olefin.

EPA requests that the submitter advise the Agency within 90 days of any modifications to its submission

EPA COMMENTS ON THE HIGHER OLEFINS CATEGORY CHALLENGE SUBMISSION

Category Definition

The category includes a non-continuous range of odd- and even-numbered mono-unsaturated olefins (C₆ through C₅₄) under 30 CAS numbers, 13 for alpha olefins and 17 for internal olefins. These CAS numbers

cover a range of substances from single compounds to complex mixtures consisting of varying proportions of linear, branched, alpha and internal olefins.

Substances Covered Under the Category "Higher Olefins"

CAS No.	Chemical Name
558-37-2	Neohexene
2437-56-1	1-Tridecene
629-73-2	1-Hexadecene (ICCA)*
112-88-9	1-Octadecene (ICCA)
3452-07-1	1-Eicosene
1599-67-3	1-Docosene
10192-32-2	1-Tetracosene
68855-58-3	Alkenes, C ₁₀₋₁₆ alpha
68855-59-4	Alkenes, C ₁₄₋₁₈ alpha
68855-60-7	Alkenes, C ₁₄₋₂₀ alpha
93924-10-8	%-Olefin fraction C ₂₀₋₂₄ cut
93924-11-9	%-Olefin fraction C ₂₄₋₂₈ cut
131459-42-2	Alkenes, C ₂₄₋₅₄ branched and linear, alpha
25264-93-1	Hexene (ICCA)
25339-56-4	Heptene (ICCA)
25377-83-7	Octene (ICCA)
27215-95-8	Nonene (ICCA)
25378-22-7	Dodecene (ICCA - not sponsored in HPV)
68526-52-3	Alkenes, C ₆
68526-53-4	Alkenes, C ₆₋₈ , C ₇ rich
68526-54-5	Alkenes, C ₇₋₉ , C ₈ rich
68526-55-6	Alkenes, C ₈₋₁₀ , C ₉ rich
68526-56-7	Alkenes, C ₉₋₁₁ , C ₁₀ rich
68526-57-8	Alkenes, C ₁₀₋₁₂ , C ₁₁ rich
68526-58-9	Alkenes, C ₁₁₋₁₃ , C ₁₂ rich
68783-10-8	Heavy polymerization naphtha (petroleum)
68991-52-6	Alkenes, C ₁₀₋₁₆
93762-80-2	Alkenes, C ₁₅₋₁₈
68514-32-9	C _{10,12} olefin rich hydrocarbons
68514-33-0	C _{12,14} olefin rich hydrocarbons

The category definition is adequate.

Category Justification

The submitter states that the incremental changes in the carbon number (C₆-C₅₄) across the category are reflected in the physicochemical/environmental properties and the toxicities of the substances. The submitter also notes that placement of the double bond within the compound and degree of branching could contribute to the physicochemical/environmental properties and toxicities of the substances. However, the available data for acute oral, repeated-dose, and reproductive toxicities show similar low toxicities for structurally diverse C₆-C₅₄ olefins. Except for some weak responses for high exposures to C₆ olefins, no mutagenicity was seen. The submitter proposed testing substances that represent the category members in the lower (C₆ internal olefins, 76% C₆ alkenes, 16% C₆ alkanes, 7% C₇ alkenes, 60-74% branched) and upper (C₂₀₋₂₄ internal olefins, 40% branched) carbon number ranges. To test the category hypothesis, the results of this proposed testing will be compared with available data for other category members.

While EPA agrees that the submitter's general approach is reasonable, there are two general areas that require further information/testing in order for the Higher Olefins category to be fully supported:

1. The submitter provided estimated values for water solubility and log K_{ow} , obtained from the ECOSAR estimation program for C_6 , C_7 , C_8 , C_9 , C_{10} , C_{12} , and C_{18} mixed internal olefins, C_6 , C_7 , C_8 , C_{10} , C_{12} , and C_{18} alpha and internal linear olefins and C_6 , C_7 , and C_8 branched alpha olefins (Tables 2, 3, and 4, respectively, of the test plan). The values for water solubility decrease, and for log K_{ow} increase, as the carbon number increases (C_6 through C_{18}) but all of the values are calculated. However, the higher hydrophobic end of the series does not model well with regard to water solubility. Therefore, the submitter needs to include measured physicochemical values as much as possible in order to demonstrate the accuracy of the estimates.
2. Biodegradation of C_6 - C_{24} olefins does not appear to depend on carbon number or degree of branching; mixtures of linear and branched olefins represent both the minimum and maximum biodegradability of the eleven compounds tested (7.63–92 %). Nonetheless, since the composition of each mixture used in the biodegradation studies in the test plan is not presented, no conclusions can be drawn from the results. Based on information available in the literature, however, it is likely that the degree of branching will be the most important feature that will affect biodegradation. The submitter needs to provide information to clarify this point.

Test Plan

Chemistry (melting point, boiling point, vapor pressure, partition coefficient, and water solubility):

The submitter provided estimated values for water solubility and log K_{ow} , and proposes providing calculated data for the other physicochemical properties. The submitter also indicates that measured physicochemical data will be provided for selected product streams where readily available. In particular, boiling points (decomposition points if appropriate), water solubilities, and vapor pressures need to be measured for a representative sampling of category members. The use of estimated values introduces uncertainties that then become magnified in modeling applications. It is not sufficient to present the data in tables in the test plan (such as in Table 2, page 9). The submitter needs to provide robust summaries for each chemical and endpoint, and clearly indicate if the data are calculated or measured, and the source of the data.

Fate (photodegradation, stability in water, chemical transport and distribution in the environment, biodegradation)

EPA agrees with the submitter's approach to photodegradation and stability in water.

Fugacity. EPA agrees with the submitter's approach to this endpoint. However, when developing the fugacity model, the submitter needs to provide the assumption and data inputs to the model (see Guidance for Robust Summary preparation). When developing the model, the submitter needs to use measured input data as much as possible. The use of estimated values introduces uncertainties which then become magnified in modeling applications. Although EPA had previously recommended the use of the Level I model, this model is somewhat limited. EPA now recommends the use of the Level III model, which provides a more rigorous level of analysis.

Biodegradation. The highest molecular weight alpha olefins for which the submitter provided biodegradation data is C_{24-30} alkenes (CAS # 182636-05-1, which is not specifically covered under the proposed category). However, the data for C_{24-30} alkenes indicate that only 51% degraded in 28 days. The submitter concluded

that C₂₄₋₃₀ alkenes are not readily biodegradable under OECD Guideline 301 B. Furthermore, in Table 8 (page 22), the submitter indicates that data for 1-hexadecene and 1-octadecene (which according to the submitter are biodegradable) will be used to “read across” to the rest of the alpha olefins, which have higher molecular weights, up to C₅₄. EPA disagrees with this approach. EPA believes that any alpha olefin in the C₅₄ range is unlikely to degrade unless major actions are taken to emulsify and/or disperse the test substance. The submitter needs to provide biodegradation data (following OECD guidelines) for a representative selection of olefins with higher molecular weights (C₃₀ - C₅₄).

Health Effects (acute toxicity, repeat dose toxicity, genetic toxicity, and reproductive/developmental toxicity)

The Higher Olefins test plan is focused on testing of materials at the lower and upper ends of the series of higher olefins with comparison of the results to existing data for specific chemicals and mixtures. The materials selected for testing are a C₆ internal olefin stream and a C₁₈ mostly linear internal olefin. The C₆ internal olefin is a member of the higher olefins category. Results obtained for this material will be compared with the toxicity profile obtained for 1-hexene under the SIDS program. The C₁₈ internal olefin is not an HPV material and is not a member of the category. The submitter has justified its use on the basis that it is a component of one of the members in the category (details not provided) and represents the upper end of the series of internal olefins present in the category. The results of tests on the C₁₈ material will be compared to existing data for 1-tetradecene and C₂₀₋₂₄ mixed linear and branched internal olefins (neither material is a specified member of the category) to determine whether the materials have similar toxicity profiles. If the proposed comparisons show similar toxicity profiles, the submitter indicates that no further testing will be conducted. Alternatively, if the comparisons indicate significant differences in the toxicity profiles of the materials, a reassessment of the category will be conducted.

Generally, EPA believes that the proposed approach is acceptable provided the members of the category and non-member analogs show similar toxicities.

Acute Toxicity. The submitted data are adequate for the purposes of the HPV Challenge Program.

Repeated-Dose Toxicity. EPA agrees with the submitter's proposal for additional testing for this endpoint. None of the submitted studies were conducted on materials specifically included in the Higher Olefin category, and the submitted data are not adequate. To address this endpoint, the submitter proposes conducting an OECD Test Guideline 422 28-day combined repeated dose/reproductive/developmental toxicity screening test on a C₆ internal olefin stream (76% C₆ alkenes, 16% C₆ alkanes, 7% C₇ alkanes, 60-74% branched). The purpose of this test is to evaluate whether or not branching and/or internalization of the double bond alters the toxicity of members of this category.

Genetic Toxicity. The submitted data are adequate for the purposes of the HPV Challenge Program.

Reproductive and Developmental Toxicity. EPA agrees with the submitter's proposal to perform one study each on high and low molecular weight materials to characterize reproductive and developmental toxicity for the category. As stated above, for the low molecular weight end of the series, a 28-day combined oral repeated dose/reproductive/developmental toxicity screening test (OECD Test Guideline 422) will be conducted on a C₆ internal olefin stream. The results of this study will be compared with existing reproductive and developmental toxicity data for 1-hexene obtained from well-conducted OECD guideline studies. For the higher molecular weight materials, the submitter proposes to perform an oral reproductive/developmental toxicity screen in rats (OECD Test Guideline 421) on a C₁₈, mostly linear (20-30% branched) internal olefin. The results of this study will be compared with existing reproductive and developmental toxicity data for 1-tetradecene obtained from a well-conducted OECD guideline study. The submitter anticipates that this approach will identify differences in the toxicity profile (if any) that are attributable to internalization of the double bond or to a branched structure.

Ecological Effects (fish, invertebrates, and algae).

EPA agrees with the submitter's statement that the acute aquatic toxicities of lower-molecular-weight olefins are not influenced by the double bond position or degree of branching. To confirm this approach the submitter proposes acute invertebrate and algal toxicity testing on a C₆ internal olefin. EPA agrees with the submitter that the olefins with a carbon number >10 are insufficiently water soluble to cause acute aquatic toxicity and any acute data at this carbon chain length or greater are minimally useful. EPA recommends chronic testing in aquatic invertebrates for chemicals and mixtures predominantly containing chemicals with log K_{ow} values of ≤ 4.2 . Therefore, the submitter needs to explain why there is no proposed testing of potential chronic toxicity. EPA believes that this testing is necessary to clarify the chronic toxicity of this category.

The submitter also needs to consider testing C₁₀-rich blends using measured concentrations at or below their water solubility for the algal and invertebrate end points (as was done for fish) due to the inadequate data submitted for this member of the series.

The test plan states that for acute toxicity, the existing data (Table 5) indicate that through the C₁₀ olefins, acute toxicity can be observed in the range of the product's water solubility. EPA disagrees with this assertion, and believes that the toxicities for several endpoints have been tested above their water solubility. For this reason, additional measured data on water solubility for those substances for which testing is proposed are necessary to determine data adequacy for ecological effects.

EPA was unable to find the rainbow trout study on alkenes, C₆ (internal branched stream) reported in Table 5 after looking in submitted robust summaries in the OECD SIDS and HPV packages.

For C₈, Table 5 of the test plan reports a 24-hour daphnid EC₅₀ while the OECD SIDS robust summary reports a 48-hour EC₅₀ for the same value. The submitter needs to address this discrepancy.

Finally, some of these studies are not fully reliable because test concentrations were nominal rather than measured. In these cases, EPA may prefer to rely on values estimated from modeling such as ECOSAR, where the models are derived only from adequate studies using measured concentrations.

Specific Comments on the Robust Summaries

Health Effects: The following deficiencies were noted in most summaries: 1) the composition or purity of the test substances was not reported; 2) numerical summary data were not provided for treatment-related effects; and 3) the citations for study reports were abbreviated and did not provide information such as the full title of the report or the contract laboratory report number. Addition of this information, if available, would assist in the review and assessment of the summarized studies.

Two entries in the table of contents for the robust summaries need to be corrected. The chain length for CAS No. 27070-58-2 is incorrectly listed as C₁₀. An acute oral toxicity test is incorrectly listed in the table of contents for the robust summaries for CAS No. 68526-53-4 (C₆-C₈, C₇ rich). The robust summary provided is for an *in vivo* genotoxicity study.

Ecological Effects

Acute testing conducted on the C₁₆ and greater higher olefins was considered inadequate because these substances were tested above their estimated water solubility limits. EPA agrees with the submitter that,

owing to their very low water solubilities, these chemicals will likely show no acute or chronic effects and, therefore, need not be tested.

C₁₀₋₁₂ Olefins

Fish. A missing data element from the robust summary for the LC₅₀ value = 0.12 mg/L study is water hardness. All other data were obtained above the predicted water solubility and, therefore may be inadequate.

Follow-up Activity

EPA requests that the submitter advise the Agency within 90 days of any modifications to its submission.